Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:15 PM GMT

PDB ID	:	4EA0
Title	:	Crystal structure of dehydrosqualene synthase (Crtm) from S. aureus complexed with diphosphate and quinuclidine BPH-651
Authors	:	Lin, F.-Y.; Liu, Y.-L.; Oldfield, E.
Deposited on	:	2012-03-21
Resolution	:	2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

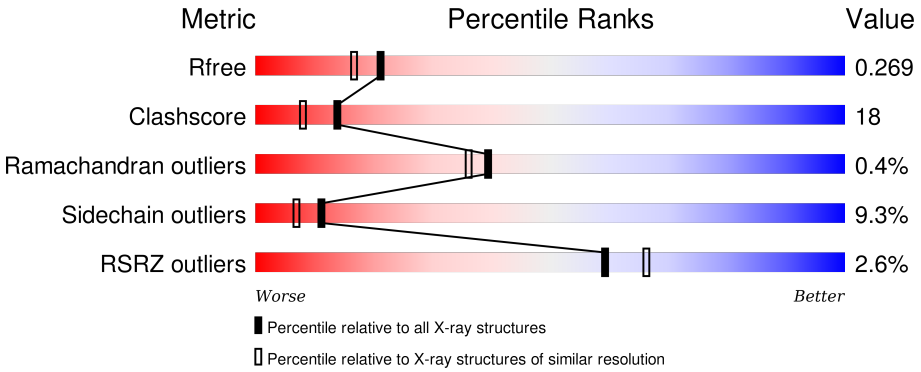
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	2% 72% 22% 5%
1	B	287	3% 66% 26% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5046 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

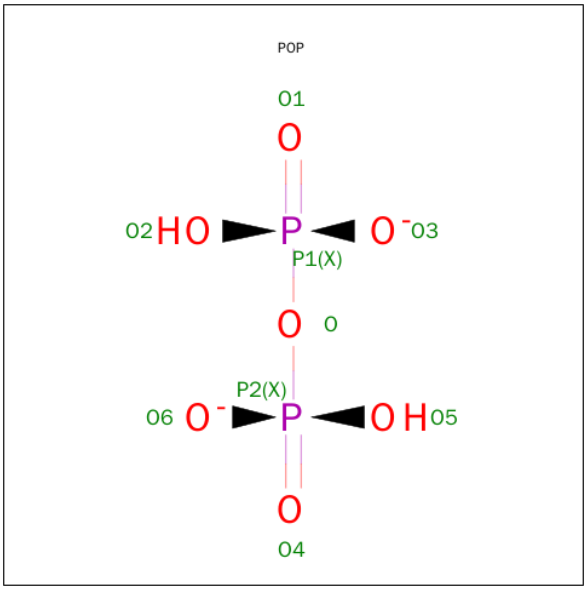
- Molecule 1 is a protein called Dehydrosqualene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2392	1536	400	444	12			
1	B	284	Total	C	N	O	S	0	0	0
			2392	1536	400	444	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

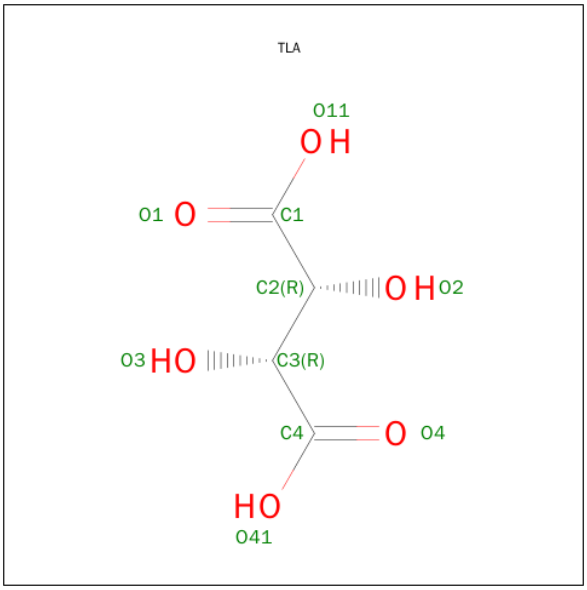
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



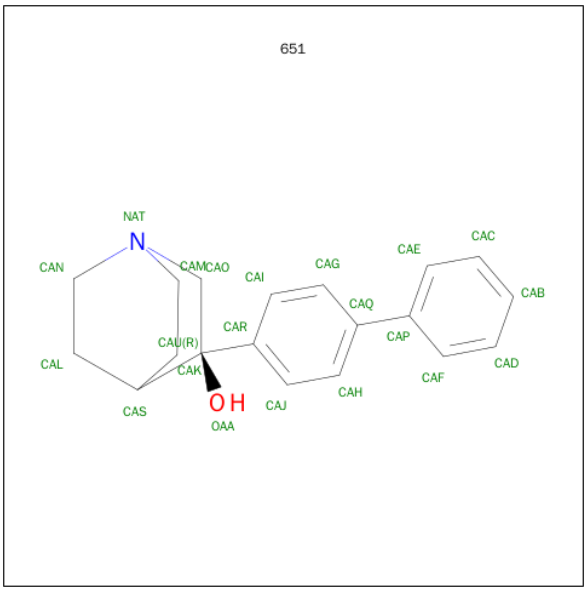
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 4 6	0	0

- Molecule 5 is (3R)-3-BIPHENYL-4-YL-1-AZABICYCLO[2.2.2]OCTAN-3-OL (three-letter code: 651) (formula: $C_{19}H_{21}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 21 19 1 1	0	0
5	B	1	Total C N O 21 19 1 1	0	0

- Molecule 6 is water.

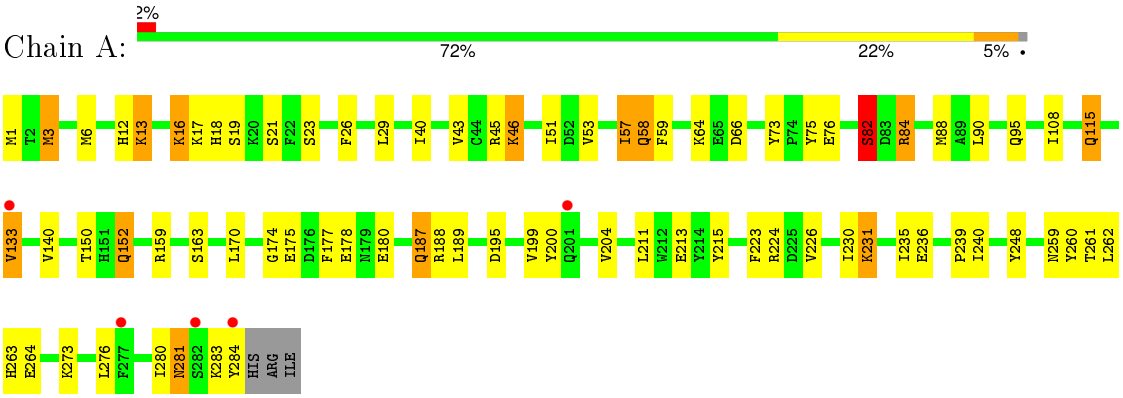
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	103	Total O 103 103	0	0
6	B	83	Total O 83 83	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

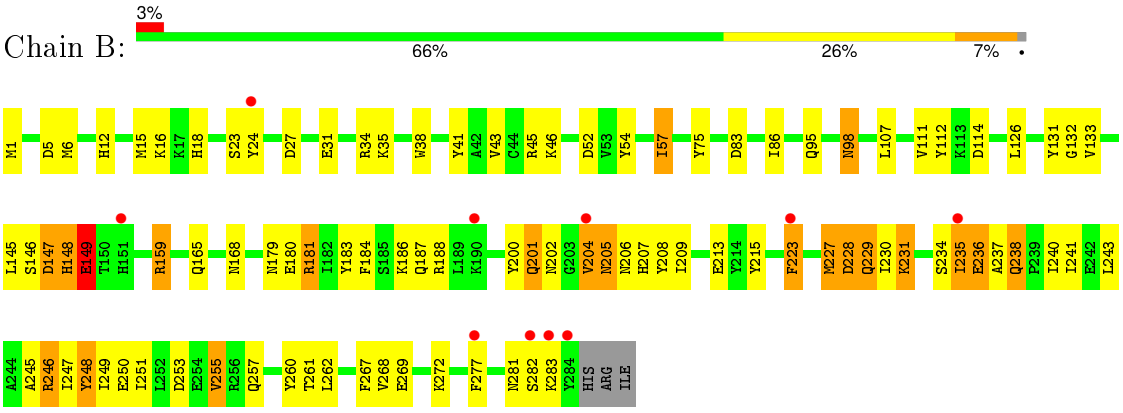
- Molecule 1: Dehydrosqualene synthase

Chain A:



- Molecule 1: Dehydrosqualene synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	80.32Å 80.32Å 180.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.46 – 2.12 32.46 – 2.12	Depositor EDS
% Data completeness (in resolution range)	94.2 (32.46-2.12) 94.2 (32.46-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.278 0.220 , 0.269	Depositor DCC
R_{free} test set	1856 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.7	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 36914 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5046	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.53 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0119e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, MG, POP, 651

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	2/2448 (0.1%)	0.45	0/3301
1	B	0.53	0/2448	0.47	1/3301 (0.0%)
All	All	0.49	2/4896 (0.0%)	0.46	1/6602 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	VAL	CB-CG1	-5.13	1.42	1.52
1	A	82	SER	CB-OG	-5.04	1.35	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	181	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2321	59	0
1	B	2392	0	2321	107	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	9	0	0	3	0
3	B	9	0	0	2	0
4	A	10	0	4	3	0
5	A	21	0	21	7	0
5	B	21	0	21	3	0
6	A	103	0	0	9	1
6	B	83	0	0	2	1
All	All	5046	0	4688	176	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:H	1:B:235:ILE:CD1	1.35	1.32
1:A:66:ASP:OD1	1:A:82:SER:HB2	1.36	1.25
1:B:235:ILE:HD13	1:B:235:ILE:N	1.48	1.17
1:B:205:ASN:OD1	1:B:207:HIS:N	1.78	1.15
1:A:3:MET:HE3	1:A:6:MET:HE1	1.06	1.04
1:B:235:ILE:N	1:B:235:ILE:CD1	2.05	1.03
1:A:3:MET:HA	1:A:6:MET:HE3	1.35	1.03
1:A:3:MET:HE3	1:A:6:MET:CE	1.89	1.02
1:A:19:SER:HA	4:A:305:TLA:H3	1.03	1.02
1:A:3:MET:CE	1:A:6:MET:HE1	1.88	1.02
1:B:227:MET:HA	1:B:227:MET:CE	1.90	1.00
1:B:227:MET:HA	1:B:227:MET:HE3	1.42	1.00
1:B:234:SER:O	1:B:238:GLN:NE2	1.97	0.97
1:A:19:SER:CA	4:A:305:TLA:H3	1.92	0.97
1:B:223:PHE:CE1	1:B:249:ILE:HD11	2.00	0.95
1:B:1:MET:HE2	1:B:6:MET:HG2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:CG	1:B:159:ARG:HH11	1.81	0.94
1:B:159:ARG:NH1	1:B:159:ARG:HB2	1.83	0.94
5:A:306:651:HAKA	6:A:501:HOH:O	1.66	0.93
1:B:148:HIS:H	1:B:148:HIS:CD2	1.85	0.92
1:A:66:ASP:OD1	1:A:82:SER:CB	2.17	0.92
1:A:19:SER:HA	4:A:305:TLA:C3	1.98	0.92
1:B:159:ARG:HH11	1:B:159:ARG:HG3	1.33	0.91
1:B:251:ILE:O	1:B:255:VAL:HG23	1.71	0.90
5:A:306:651:CAK	6:A:501:HOH:O	2.22	0.87
1:B:1:MET:CE	1:B:6:MET:HG2	2.08	0.84
1:B:148:HIS:N	1:B:148:HIS:CD2	2.44	0.82
1:B:205:ASN:OD1	1:B:206:ASN:N	2.12	0.82
1:A:3:MET:HA	1:A:6:MET:CE	2.08	0.82
1:B:223:PHE:CD1	1:B:249:ILE:HD11	2.17	0.80
1:B:235:ILE:H	1:B:235:ILE:HD13	0.65	0.79
1:A:195:ASP:O	1:A:199:VAL:HG23	1.83	0.79
1:B:234:SER:C	1:B:238:GLN:HE22	1.87	0.77
1:B:253:ASP:O	1:B:257:GLN:HG3	1.85	0.76
5:A:306:651:OAA	5:A:306:651:HAN	1.86	0.76
1:A:3:MET:CE	1:A:6:MET:CE	2.54	0.75
1:B:159:ARG:NH1	1:B:159:ARG:CB	2.50	0.74
1:A:213:GLU:O	6:A:463:HOH:O	2.07	0.72
5:B:305:651:HAN	5:B:305:651:OAA	1.88	0.72
1:B:205:ASN:OD1	1:B:205:ASN:C	2.30	0.70
1:B:148:HIS:H	1:B:148:HIS:HD2	1.37	0.70
1:B:159:ARG:HH11	1:B:159:ARG:CB	2.04	0.69
1:B:148:HIS:N	1:B:148:HIS:HD2	1.89	0.69
1:B:251:ILE:O	1:B:255:VAL:CG2	2.40	0.69
5:A:306:651:OAA	5:A:306:651:CAN	2.30	0.69
1:A:204:VAL:O	1:A:204:VAL:HG23	1.94	0.66
1:A:200:TYR:CE1	1:A:263:HIS:CE1	2.84	0.65
1:B:228:ASP:O	1:B:231:LYS:NZ	2.30	0.65
5:B:305:651:CAN	5:B:305:651:OAA	2.39	0.63
1:A:12:HIS:CD2	1:A:16:LYS:HD3	2.34	0.63
1:B:248:TYR:O	1:B:251:ILE:HB	2.00	0.61
1:A:224:ARG:NH2	6:A:474:HOH:O	2.20	0.61
1:B:235:ILE:N	1:B:235:ILE:HD12	2.08	0.60
1:B:204:VAL:HG11	1:B:260:TYR:HB2	1.83	0.60
1:A:235:ILE:H	1:A:235:ILE:HD12	1.66	0.60
1:B:230:ILE:HG13	1:B:230:ILE:O	2.01	0.60
1:B:227:MET:HA	1:B:227:MET:HE2	1.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:O	1:A:280:ILE:HG12	2.01	0.60
1:B:184:PHE:CD1	1:B:215:TYR:CE2	2.90	0.60
1:B:159:ARG:HB2	1:B:159:ARG:HH11	1.61	0.59
1:B:1:MET:HG3	1:B:5:ASP:HB2	1.86	0.57
1:A:17:LYS:HD2	1:A:17:LYS:O	2.05	0.56
1:A:13:LYS:HA	1:A:16:LYS:HE2	1.88	0.56
1:B:204:VAL:HG12	1:B:208:TYR:CD2	2.41	0.55
1:A:51:ILE:HD12	1:A:115:GLN:HG3	1.88	0.55
1:A:73:TYR:HB3	1:A:76:GLU:HG2	1.87	0.55
1:B:227:MET:O	1:B:230:ILE:HG22	2.07	0.55
1:A:235:ILE:N	1:A:235:ILE:HD12	2.22	0.55
1:B:223:PHE:CZ	1:B:249:ILE:HD11	2.42	0.55
1:B:52:ASP:HB2	6:B:482:HOH:O	2.06	0.55
1:B:236:GLU:CD	1:B:236:GLU:H	2.03	0.54
1:A:46:LYS:HZ3	1:A:59:PHE:HZ	1.53	0.54
1:A:84:ARG:O	1:A:88:MET:HG2	2.08	0.53
1:B:45:ARG:HH22	3:B:304:POP:P2	2.30	0.53
1:B:237:ALA:HB1	1:B:241:ILE:HD12	1.91	0.53
1:B:246:ARG:HA	1:B:249:ILE:HD12	1.91	0.53
1:B:238:GLN:H	1:B:238:GLN:HE21	1.58	0.52
1:B:148:HIS:O	1:B:149:GLU:C	2.46	0.52
1:B:245:ALA:O	1:B:249:ILE:HG13	2.09	0.52
1:B:268:VAL:HG12	1:B:272:LYS:HB3	1.90	0.52
1:B:223:PHE:CE1	1:B:249:ILE:CD1	2.84	0.52
1:A:204:VAL:O	1:A:204:VAL:CG2	2.57	0.52
1:B:236:GLU:N	1:B:236:GLU:OE2	2.23	0.51
1:B:243:LEU:O	1:B:247:ILE:HG13	2.12	0.50
1:A:75:TYR:CE1	1:A:95:GLN:HG2	2.47	0.50
1:B:148:HIS:O	1:B:149:GLU:O	2.30	0.50
1:B:43:VAL:CG2	1:B:86:ILE:CG2	2.90	0.50
1:B:236:GLU:O	1:B:240:ILE:HD12	2.12	0.50
1:A:239:PRO:HD3	1:A:284:TYR:CE2	2.47	0.50
1:B:75:TYR:CE1	1:B:95:GLN:HG2	2.47	0.50
1:A:189:LEU:HD23	1:A:211:LEU:CD2	2.42	0.50
1:B:159:ARG:CG	1:B:159:ARG:NH1	2.50	0.49
1:A:281:ASN:O	1:A:284:TYR:O	2.30	0.49
1:B:179:ASN:O	1:B:180:GLU:HB2	2.11	0.49
1:A:18:HIS:CB	1:A:45:ARG:HD3	2.42	0.49
1:B:159:ARG:NH1	1:B:159:ARG:HG3	2.14	0.49
1:A:236:GLU:H	1:A:236:GLU:CD	2.15	0.49
1:A:187:GLN:OE1	1:A:188:ARG:CZ	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:HIS:CB	1:B:45:ARG:HD3	2.43	0.48
1:B:227:MET:CE	1:B:227:MET:CA	2.70	0.48
3:A:304:POP:O	5:A:306:651:CAM	2.62	0.48
1:B:12:HIS:HB2	1:B:38:TRP:CE3	2.48	0.48
3:A:304:POP:O3	6:A:503:HOH:O	2.18	0.48
1:B:234:SER:C	1:B:238:GLN:NE2	2.54	0.48
1:B:200:TYR:HA	1:B:262:LEU:HD22	1.97	0.47
1:B:1:MET:HG3	1:B:5:ASP:CB	2.44	0.47
1:B:1:MET:HE3	1:B:6:MET:HA	1.97	0.47
1:A:170:LEU:HD21	1:A:215:TYR:HB2	1.96	0.46
1:B:201:GLN:HG3	1:B:202:ASN:OD1	2.15	0.46
1:A:3:MET:HE2	1:A:6:MET:HE3	1.97	0.46
1:A:235:ILE:H	1:A:235:ILE:CD1	2.28	0.46
1:A:3:MET:CE	1:A:6:MET:HE3	2.42	0.46
5:A:306:651:HAK	6:A:501:HOH:O	2.01	0.46
1:A:46:LYS:NZ	1:A:59:PHE:HZ	2.14	0.46
1:A:261:THR:HG21	1:A:264:GLU:HG3	1.96	0.46
1:B:107:LEU:HA	1:B:132:GLY:O	2.15	0.46
1:B:43:VAL:HG22	1:B:86:ILE:CG2	2.46	0.46
1:B:15:MET:HA	1:B:41:TYR:CE1	2.50	0.46
1:B:52:ASP:CB	6:B:482:HOH:O	2.64	0.46
1:B:229:GLN:HA	1:B:231:LYS:NZ	2.31	0.46
1:B:186:LYS:O	1:B:187:GLN:C	2.55	0.46
1:B:223:PHE:CZ	1:B:249:ILE:CD1	2.99	0.45
1:B:126:LEU:HD13	1:B:183:TYR:O	2.16	0.45
1:B:43:VAL:HG22	1:B:86:ILE:HG22	1.99	0.45
1:B:209:ILE:O	1:B:213:GLU:HG2	2.16	0.45
1:A:16:LYS:HB2	1:A:16:LYS:HE3	1.60	0.45
1:A:177:PHE:O	1:A:180:GLU:N	2.34	0.45
1:B:205:ASN:HD21	1:B:207:HIS:HB2	1.82	0.45
1:B:43:VAL:HG23	1:B:86:ILE:CG2	2.47	0.45
1:B:31:GLU:O	1:B:35:LYS:HG3	2.16	0.44
1:A:21:SER:HA	1:A:273:LYS:HE2	1.99	0.44
1:B:146:SER:HA	1:B:234:SER:HB3	2.00	0.44
1:A:236:GLU:O	1:A:240:ILE:HD13	2.17	0.44
1:A:57:ILE:HD13	1:A:57:ILE:C	2.38	0.44
1:B:1:MET:HE3	1:B:6:MET:HG2	1.95	0.44
1:A:231:LYS:HA	1:A:231:LYS:HD3	1.52	0.44
1:A:260:TYR:O	1:A:262:LEU:HD12	2.17	0.44
1:B:269:GLU:HG3	1:B:269:GLU:H	1.66	0.44
1:B:188:ARG:HD3	1:B:188:ARG:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG21	1:A:90:LEU:HD22	1.99	0.44
1:A:150:THR:OG1	1:A:152:GLN:HG2	2.17	0.44
1:A:64:LYS:HB2	1:A:108:ILE:HD13	1.99	0.44
1:B:165:GLN:O	1:B:168:ASN:HB3	2.18	0.44
1:B:248:TYR:HA	1:B:251:ILE:HD12	1.99	0.43
1:B:16:LYS:HG3	1:B:23:SER:OG	2.18	0.43
1:A:174:GLY:O	1:A:178:GLU:HG3	2.18	0.43
1:B:111:VAL:O	1:B:114:ASP:HB2	2.18	0.43
1:B:145:LEU:O	1:B:146:SER:OG	2.32	0.43
1:B:83:ASP:CG	1:B:86:ILE:HD12	2.37	0.43
1:B:246:ARG:NH1	1:B:250:GLU:OE1	2.45	0.43
1:B:213:GLU:OE2	1:B:260:TYR:OH	2.23	0.43
1:B:184:PHE:CE1	1:B:215:TYR:CD2	3.06	0.43
1:B:41:TYR:CD1	1:B:41:TYR:C	2.93	0.42
1:B:268:VAL:CG1	1:B:272:LYS:HB3	2.48	0.42
1:A:53:VAL:HG21	1:B:54:TYR:OH	2.19	0.42
3:A:304:POP:O	5:A:306:651:HAMA	2.19	0.42
1:A:259:ASN:OD1	6:A:497:HOH:O	2.21	0.42
1:B:46:LYS:HG3	1:B:86:ILE:HD13	2.02	0.42
1:B:231:LYS:H	1:B:231:LYS:HG3	1.57	0.42
3:B:304:POP:O	5:B:305:651:CAM	2.68	0.41
1:B:24:TYR:C	1:B:24:TYR:CD2	2.93	0.41
1:A:159:ARG:HG2	1:A:226:VAL:CG2	2.51	0.41
1:B:237:ALA:HB1	1:B:241:ILE:CD1	2.50	0.41
1:B:229:GLN:HA	1:B:231:LYS:HZ2	1.84	0.41
1:A:26:PHE:HD1	1:A:29:LEU:HD11	1.86	0.41
1:B:57:ILE:HG13	1:B:112:TYR:HE1	1.86	0.41
1:A:40:ILE:HD13	1:A:140:VAL:HG12	2.03	0.41
1:A:13:LYS:HE3	6:A:478:HOH:O	2.20	0.40
1:B:237:ALA:O	1:B:238:GLN:C	2.59	0.40
1:B:159:ARG:CZ	1:B:159:ARG:CB	2.98	0.40
1:A:46:LYS:HD2	1:A:46:LYS:HA	1.72	0.40
1:B:98:ASN:ND2	1:B:98:ASN:C	2.75	0.40
1:B:243:LEU:HD22	1:B:277:PHE:CD2	2.56	0.40
1:B:27:ASP:O	1:B:34:ARG:NH1	2.55	0.40
1:B:147:ASP:OD1	1:B:147:ASP:N	2.53	0.40
1:A:58:GLN:HB2	6:A:484:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:459:HOH:O	6:B:448:HOH:O[4_545]	2.07	0.13

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/287 (98%)	271 (96%)	10 (4%)	1 (0%)	39	36
1	B	282/287 (98%)	261 (93%)	20 (7%)	1 (0%)	39	36
All	All	564/574 (98%)	532 (94%)	30 (5%)	2 (0%)	39	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	GLU
1	A	82	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/260 (99%)	236 (92%)	21 (8%)	14	10
1	B	257/260 (99%)	230 (90%)	27 (10%)	8	5
All	All	514/520 (99%)	466 (91%)	48 (9%)	11	7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	MET
1	A	13	LYS
1	A	16	LYS
1	A	23	SER
1	A	46	LYS
1	A	57	ILE
1	A	58	GLN
1	A	84	ARG
1	A	115	GLN
1	A	133	VAL
1	A	152	GLN
1	A	163	SER
1	A	175	GLU
1	A	187	GLN
1	A	223	PHE
1	A	230	ILE
1	A	231	LYS
1	A	248	TYR
1	A	281	ASN
1	A	283	LYS
1	B	57	ILE
1	B	98	ASN
1	B	133	VAL
1	B	147	ASP
1	B	148	HIS
1	B	149	GLU
1	B	159	ARG
1	B	181	ARG
1	B	201	GLN
1	B	204	VAL
1	B	205	ASN
1	B	223	PHE
1	B	227	MET
1	B	228	ASP
1	B	229	GLN
1	B	231	LYS
1	B	235	ILE
1	B	236	GLU
1	B	238	GLN
1	B	246	ARG
1	B	248	TYR
1	B	255	VAL

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Mol	Chain	Res	Type
1	B	261	THR
1	B	267	PHE
1	B	281	ASN
1	B	282	SER
1	B	283	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	96	HIS
1	A	281	ASN
1	B	98	ASN
1	B	148	HIS
1	B	238	GLN
1	B	257	GLN
1	B	263	HIS
1	B	281	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	POP	A	304	2	8,8,8	0.59	0	13,13,13	1.48	1 (7%)
4	TLA	A	305	-	3,9,9	0.77	0	6,12,12	1.96	1 (16%)
5	651	A	306	-	23,24,24	3.18	5 (21%)	29,35,35	1.80	6 (20%)
3	POP	B	304	2	8,8,8	0.55	0	13,13,13	1.33	1 (7%)
5	651	B	305	-	23,24,24	2.38	4 (17%)	29,35,35	1.52	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	A	304	2	-	0/6/6/6	0/0/0/0
4	TLA	A	305	-	-	0/4/12/12	0/0/0/0
5	651	A	306	-	-	0/10/31/31	0/2/4/4
3	POP	B	304	2	-	0/6/6/6	0/0/0/0
5	651	B	305	-	-	0/10/31/31	0/2/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	651	CAU-CAS	-12.84	1.43	1.54
5	B	305	651	CAU-CAS	-8.91	1.47	1.54
5	B	305	651	CAQ-CAP	-4.65	1.36	1.49
5	A	306	651	CAQ-CAP	-4.13	1.38	1.49
5	A	306	651	CAO-NAT	-4.01	1.41	1.46
5	B	305	651	CAO-NAT	-3.16	1.42	1.46
5	A	306	651	CAU-CAR	-3.07	1.49	1.52
5	A	306	651	CAK-CAS	-3.03	1.44	1.53
5	B	305	651	CAK-CAS	-2.90	1.45	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	306	651	CAM-NAT-CAO	-6.52	100.36	109.40
3	A	304	POP	P2-O-P1	-4.51	120.08	132.73
4	A	305	TLA	C4-C3-C2	-4.03	105.08	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	304	POP	P2-O-P1	-3.94	121.67	132.73
5	A	306	651	CAF-CAP-CAQ	-3.09	115.84	121.39
5	B	305	651	CAM-NAT-CAO	-3.08	105.14	109.40
5	B	305	651	CAM-CAK-CAS	-2.92	104.23	110.79
5	B	305	651	CAE-CAP-CAQ	-2.70	116.55	121.39
5	A	306	651	CAM-CAK-CAS	-2.56	105.03	110.79
5	A	306	651	CAJ-CAR-CAU	-2.28	117.88	121.06
5	B	305	651	CAH-CAJ-CAR	-2.06	118.53	121.26
5	B	305	651	CAL-CAN-NAT	-2.06	107.60	110.96
5	A	306	651	CAO-CAU-CAS	2.16	112.76	108.46
5	A	306	651	CAE-CAP-CAQ	2.21	125.36	121.39
5	B	305	651	CAF-CAP-CAQ	2.22	125.37	121.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	POP	3	0
4	A	305	TLA	3	0
5	A	306	651	7	0
3	B	304	POP	2	0
5	B	305	651	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	284/287 (98%)	0.08	5 (1%) 71 76	24, 42, 64, 87	0
1	B	284/287 (98%)	0.08	10 (3%) 48 57	25, 48, 71, 104	0
All	All	568/574 (98%)	0.08	15 (2%) 59 66	24, 44, 69, 104	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	TYR	5.5
1	A	282	SER	3.6
1	B	277	PHE	3.3
1	B	282	SER	3.1
1	A	284	TYR	3.1
1	B	223	PHE	3.0
1	A	277	PHE	2.7
1	B	190	LYS	2.6
1	A	133	VAL	2.4
1	A	201	GLN	2.4
1	B	283	LYS	2.4
1	B	24	TYR	2.4
1	B	204	VAL	2.1
1	B	151	HIS	2.0
1	B	235	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	TLA	A	305	10/10	0.79	0.18	1.17	47,57,62,63	0
2	MG	B	302	1/1	0.99	0.12	1.10	33,33,33,33	0
2	MG	A	303	1/1	0.99	0.12	0.91	29,29,29,29	0
5	651	B	305	21/21	0.91	0.18	0.82	33,39,44,48	0
2	MG	A	302	1/1	0.98	0.18	0.75	23,23,23,23	0
5	651	A	306	21/21	0.84	0.18	0.44	26,35,42,52	0
3	POP	A	304	9/9	0.99	0.15	0.09	25,27,28,30	0
2	MG	B	301	1/1	0.99	0.11	-0.13	29,29,29,29	0
3	POP	B	304	9/9	0.98	0.11	-0.18	26,31,35,37	0
2	MG	A	301	1/1	0.99	0.16	-	34,34,34,34	0
2	MG	B	303	1/1	0.95	0.09	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.